? t s2/7/4,5,28,35,36,38,53

2/7/4 (Item 4 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

08649019 96302261
Raman spectroscopy of the Ff gene V protein and complexes with poly(dA): nonspecific DNA recognition and binding.
Benevides JM; Terwilliger TC; Vohnik S; Thomas GJ Jr
Division of Cell Biology and Biophysics, School of Biological Sciences, University of Missouri-Kansas City 64110, USA.
Biochemistry (UNITED STATES) Jul 23 1996, 35 (29) p9603-9, ISSN 0006-2960 Journal Code: A0G
Contract/Grant No.: GM50776, GM, NIGMS
Languages: ENGLISH
Document type: JOURNAL ARTICLE
Raman spectra of crystals and solutions of the single-stranded DNA binding protein of bacteriophage Ff (gene V protein, gVp) and of solution complexes of gVp with single-stranded poly-(deoxyadenylic acid) [poly(dA)] reveal the following: (i) The gVp secondary and tertiary structures are similar in solution and in the crystal and are dominated by beta-sheet domains, in agreement with NMR and X-ray findings. (ii) Subunit conformation and side chain environments of gVp are virtually unchanged over a wide range of salt concentration (0 < [NaCl] < 100 mM); however, the solution conformation of poly(dA) exhibits sensitivity to added salt. The perturbed Raman markers indicate subtle changes in helix backbone geometry with accompanying small differences in base stacking as the concentration of NaCl is changed. (iii) In complexes with poly(dA), neither the conformation of gVp nor its side chain environments are altered significantly in comparison to the free protein. This is the case at both high salt (nucleotide-to-subunit binding stoichiometry n = 4) and low salt (n = 3). (iv) The Raman signature of poly(dA) undergoes small perturbations upon gVp binding, indicative of small changes in base stacking and phosphodiester backbone conformation. The present results show that the different stoichiometric binding modes of gVp to poly(dA) are accomplished without significant changes in gVp subunit structure and with only modest changes in the single-stranded poly(dA) ligand. This contrasts sharply with sequence-specific double-stranded DNA binding proteins, such as the phage lambda and D108 repressors, which undergo substantial structural changes upon DNA binding, and which also alter more dramatically the Raman fingerprints of their DNA target sites. Thus, nonspecific and specific nucleic acid recognition modes are distinguishable by Raman spectroscopy. The Raman signature of gVp also allows examination of hydrogen bonding interactions of unique side chains within the hydrophobic core (cysteine 33) and at the binding interface (tyrosine 41). These are discussed in relation to the recently published gVp crystal structure.

2/7/5 (Item 5 from file: 155)
DIALOG(R)File 155:MEDLINE(R)

08413453 95272432
Raman spectroscopy of DNA and proteins.
Peticolas WL
Department of Chemistry, University of Oregon, Eugene 97403, USA.
Methods Enzymol (UNITED STATES) 1995, 246 p389-416, ISSN 0076-6879 Journal Code: MVA

Languages: ENGLISH
Document type: JOURNAL ARTICLE

2/7/28 (Item 1 from file: 434)
DIALOG(R)File 434:Scisearch(R) Cited Ref Sci

14978723 Genuine Article#: VA608 Number of References: 24
Title: RATIONAL DESIGN OF FIBEROPTIC PROBES FOR VISIBLE AND PULSED-ULTRAVIOLET RESONANCE RAMAN-SPECTROSCOPY
Author(s): GREEK LS; SCHULZE HG; HAYNES CA; BLADES MW; TURNER RFB
Corporate Source: UNIV BRITISH COLUMBIA,BIOTECHNOL LAB,237-6174 UNIV BLVD/VANCOUVER/BC V6T 1Z3/CANADA/; UNIV BRITISH COLUMBIA,DEPT PSYCHOL/VANCOUVER/BCV6T 1Z1/CANADA/; UNIV BRITISH COLUMBIA,DEPT CHEM/VANCOUVER/BC V6T 1Z1/CANADA/; UNIV BRITISH COLUMBIA,DEPT ELECT ENGN/VANCOUVER/BC V6T 1Z4/CANADA/; UNIV BRITISH COLUMBIA,DEPT CHEM ENGN/VANCOUVER/BC V6T 1Z4/CANADA/
Journal: APPLIED OPTICS, 1996, V35, N21 (JUL 20), P4086-4095
ISSN: 0003-6935
Language: ENGLISH Document Type: ARTICLE
Abstract: The investigated the performance of fiber-optic resonance Raman probes with a series of experiments to determine the working curves of such probes using model analytes and to investigate the effects of absorbing media. A computer model designed to simulate these experiments is presented, and numerical results are found to be in agreement with the experimental data. Design considerations resulting from these studies are discussed, and novel designs for overcoming problems of coupling efficiency, damage threshold, and sensitivity in absorbing samples are presented. These findings are applied to the design of fiber-optic probes for ultraviolet resonance Raman spectroscopy involving nanosecond pulsed-ultraviolet excitation (225 and 266 nm). These probes have been used to collect what is, to our knowledge, the first reported fiber-optic-linked ultraviolet resonance Raman spectra of tryptophan and DNA. (C) 1996 Optical Society of America

2/7/35 (Item 8 from file: 434)
DIALOG(R)File 434:Scisearch(R) Cited Ref Sci

11290400 Genuine Article#: GY135 Number of References: 39
Title: STUDIES OF VIRUS STRUCTURE BY LASER RAMAN-SPECTROSCOPY .34. RAMAN-SPECTROSCOPY OF FILAMENTOUS BACTERIOPHAGE-FF (FD, M13, F1) INCORPORATING SPECIFICALLY-DEUTERATED ALANINE AND TRYPTOPHAN SIDE-CHAINS - ASSIGNMENTS AND STRUCTURAL INTERPRETATION
Author(s): AUBREY KL; THOMAS GJ
Corporate Source: UNIV MISSOURI,SCH BASIC LIFE SCI,DIV CELL BIOL & BIOPHYS/KANSAS CITY//MO/64110; UNIV MISSOURI,SCH BASIC LIFE SCI,DIV CELL BIOL & BIOPHYS/KANSAS CITY//MO/64110
Journal: BIOPHYSICAL JOURNAL, 1991, V60, N6 (DEC), P1337-1349
Language: ENGLISH Document Type: ARTICLE
Abstract: Structural interpretation of the Raman spectra of filamentous bacteriophages is dependent upon reliable assignments for the numerous Raman vibrational bands contributed from coat protein and packaged DNA of the virion. To establish unambiguous assignments and facilitate structural conclusions derived from them, we have initiated a systematic study of filamentous bacteriophage Ff (fd, f1, M13) incorporating protein subunits with specifically deuterated amino-acid

side chains. Here, we report and interpret the Raman spectra of fd virions which incorporate: (a) a single deuterio-tryptophan residue per coat protomer [fd(W(d5))], (b) ten deuterio-alanines per protomer [fd(10A(d3))], and (c) both deuterio-tryptophan and deuterio-alanine [fd(W(d5) + 10A(d3))]. The unambiguous assignment of coat protein Raman bands in normal and deuterated isotopomers of fd establishes the validity of earlier empirical assignments of many key Raman markers, including those of packaged ssDNA (Thomas et al., 1988). Present results confirm that deoxyguanosine residues of the packaged ssDNA molecule depart from the usual C2'-endo/anti conformation characteristic of protein-free DNA in aqueous solution, although C2'-endo/anti conformers of thymidine are not excluded by the data. The combined results obtained here on normal fd, and on fd incorporating deuterio-tryptophan [fd(W(d5)) and fd(W(d5) + 10A(d3))], show also that the microenvironment of the single tryptophan residue per coat protomer (W26) can be clearly deduced as follows: (a) The indole 1-NH donor group of each protomer in fd forms a moderately strong hydrogen bond, most likely to a hydroxyl oxygen acceptor. (b) The planar indole ring exists in a hydrophilic environment. (c) The torsion angle describing the orientation of the indole ring (C3-C2 linkage) with respect to the side-chain (C-alpha-C-beta bond) is unusually large, i.e., \X2,1\ approximately 120-degrees. With respect to alanine isotopomers, the present results show that alanine residues, and possibly other methyl-containing side chains, are significant contributors to the fd Raman spectrum. The present study provides new information on protomer side chains of fd and demonstrates a Raman methodology which should be generally useful for investigating single-site interactions and macromolecular conformations in other nucleoprotein assemblies.

2/7/36 (Item 9 from file: 434)
DIALOG(R)File 434:Scisearch(R) Cited Ref Sci

10908061 Genuine Article#: FR446 Number of References: 49
Title: RAMAN SPECTRAL STUDIES OF NUCLEIC-ACIDS .42. DNA RECOGNITION BY THE HELIX-TURN-HELIX MOTIF - INVESTIGATION BY LASER RAMAN-SPECTROSCOPY OF THE PHAGE LAMBDA REPRESSOR AND ITS INTERACTION WITH OPERATOR SITES OL1 AND OR3
Author(s): BENEVIDES JM; WEISS MA; THOMAS GJ
Corporate Source: UNIV MISSOURI,SCH BASIC LIFE SCI,DIV CELL BIOL & BIOPHYS/KANSAS CITY//MO/64110; UNIV MISSOURI,SCH BASIC LIFE SCI,DIV CELL BIOL & BIOPHYS/KANSAS CITY//MO/64110; HARVARD UNIV,SCH MED,DEPT BIOL CHEM & MOLEC PHARMACOL/BOSTON//MA/02115
Journal: BIOCHEMISTRY, 1991, V30, N24, P5955-5963
Language: ENGLISH Document Type: ARTICLE
Abstract: The lambda-repressor provides a model system for biophysical studies of DNA recognition by the helix-turn-helix motif. We describe laser Raman studies of the lambda-operator sites O(L)1 and O(R)3 and their interaction with the DNA-binding domain of X repressor (residues 1-102). Raman spectra of the two DNA sites exhibit significant differences attributable to interstrand purine-purine steps that differ in the two oligonucleotides. Remarkably, the conformation of each operator is significantly and specifically altered by repressor binding. Protein recognition, which involves hydrogen-bond formation and hydrophobic contacts in the major groove, induces subtle changes in DNA Raman bands of interacting groups. These include (i) site-specific perturbations to backbone phosphodiester geometry at AT-rich domains, (ii) hydrophobic interaction at thymine 5CH3 groups, (iii) hydrogen

bonding to guanine 7N and 6C = O acceptors, and (iv) alterations in sugar pucker within the C2'-endo (B-DNA) family. These perturbations differ between aqueous O(L)1 and O(R)3 complexes of repressor, indicating that protein binding in solution determines the precise DNA conformation. The overall structure of the lambda-domain is not greatly perturbed by binding to either O(L)1 or O(R)3, in accord with X-ray studies of other complexes. However, Raman markers indicate a change in hydrogen bonding of the OH group of tyrosine-22, which is a hydrogen-bond acceptor in the absence of DNA but a combined donor and acceptor in the O(L)1 complex; yet, Y22 hydrogen bonding is not altered in forming the O(R)3 complex. The present results demonstrate qualitatively different and distinguishable modes of interaction of the X repressor DNA-binding domain with operators O(L)1 and O(R)3 in solution. This application of laser Raman spectroscopy to a well-characterized system provides a prototype for future Raman studies of other DNA-binding motifs under physiological conditions.

2/7/38 (Item 11 from file: 434)
DIALOG(R)File 434:Scisearch(R) Cited Ref Sci

07452109 Genuine Article#: D5226 Number of References: 31
Title: SURFACE-ENHANCED RAMAN-SPECTROSCOPY OF AMINO-ACIDS AND NUCLEOTIDE BASES ADSORBED ON SILVER
Author(s): SUH JS; MOSKOVITS M
Corporate Source: UNIV TORONTO,DEPT CHEM/TORONTO M5S 1A1/ONTARIO/CANADA/
Journal: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 1986, V108, N16, P 4711-4718
Language: ENGLISH Document Type: ARTICLE

2/7/53 (Item 2 from file: 654)
DIALOG(R)File 654:US Pat.Full.

02124584
Utility
MIXED LIGAND COMPLEXES AND USES THEREOF AS BINDING AGENTS AND PROBES TO DNA [Spectroscopically or photoactively determinable]

PATENT NO.: 5,157,032
ISSUED: October 20, 1992 (19921020)
INVENTOR(s): Barton, Jacqueline K., San Marino, CA (California), US (United States of America)
ASSIGNEE(s): The Trustees of Columbia University In The City of New York, (A U.S. Company or Corporation), New York, NY (New York), US (United States of America)
[Assignee Code(s): 8871]
APPL. NO.: 7-539,930
FILED: June 18, 1990 (19900618)
DISCLAIMER: May 12, 2009 (20090512)

This application is a continuation-in-part of Ser. No. 268,247, filed Nov. 7, 1988, now U.S. Pat. No. 5,112,974 which is a continuation in part of U.S. Ser. No. 905,295 now abandoned filed Sept. 8, 1986, which in turn is a continuation-in-part of U.S. Ser. No. 693,023, filed Jan. 18, 1985, now U.S. Pat. No. 4,721,669, issued Jan. 26, 1988, the contents of which are hereby incorporated by reference into the present application.

The invention was made with government support under grant number CG 33309 from the National Institutes of General Medical Science, the U.S. Department of Health and Human Services and with the support from the National Science Foundation.

FULL TEXT: 2996 lines

ABSTRACT

This invention concerns a coordination complex or salt thereof which is spectroscopically or photoactively determinable when bound to DNA having the formula [See structure in original document] wherein M is a suitable transition metal and each of R sub 1, R sub 2 and R sub 3 is ethylenediamine, bipyridine, phenanthroline, diazafluorene-9-one or a substituted derivative thereof, or phenanthrenequinonediimine or a substituted derivative thereof, dypyridophenazine or a substituted derivative thereof; wherein R sub 1, R sub 2 and R sub 3 are bound to M by coordination bonds; provided that at least one of R1, R2 or R3 is dypyridophenazine or a substituted derivative thereof. The invention also concerns a labeled DNA probe which comprises the complex covalently bound to the DNA probe. Further the invention concerns a method of detecting the presence in a sample a target DNA of interest which comprises contacting the sample containing the target DNA with a complementary labeled DNA probe under hybridizing conditions and measuring the resulting luminescense emitted from the labeled DNA probe, a change in the luminescense as compared with the luminescense in the absence of the sample indicating the presence of the target DNA.

What is claimed is:

1. A coordination complex or salt thereof which is spectroscopically or photoactively determinable when bound to DNA having the formula [See structure in original document] wherein M is Ru, Rh, Co, Fe, Cr, Cu, Zn, Cd, or Pb, and each of R sub 1, R sub 2, and R sub 3 is ethylenediamine, bipyridine, 2,2'-bipyridine (bpy), 4,4'diphenyl bipyridine, bis 4,4' methyl bipyridylate, bis 4,4' bipyridylamide, phenanthroline, 1,10-phenanthroline (phen), 4,7-diamino-1,10-phenanthroline, 3,8-diamino-1,10-phenanthroline, 4,7-diethylenediamine-1,10-phenanthroline, 3,8-diethylenediamine-1,10-phenanthroline, 4,7-dihydroxyl-1,10-phenanthroline, 3,8-dihydroxyl-1,10-phenanthroline, 4,7-dinitro-1,10-phenanthroline, 3,8-dinitro-1,10-phenanthroline, 4,7-diphenyl-1,10-phenanthroline (DIP), 3,8-diphenyl-1,10-phenanthroline, 4,7-dispermine-1,10-phenanthroline, 3,8-dispermine-1,10-phenanthroline, 5-nitrophenanthroline (5-NO sub 2 phen), 3,4,7,8-tetramethyl-phenanthroline (TMP), diazafluorene-9-one, 4,5-diazafluorene-9-one (flone), phenanthrenequinonediimine, 9,10-phenanthrenequinonediimine (phi), dipyridophenanzine, or 3,2-dipyridophenazine (dppz); wherein R sub 1, R sub 2, and R sub 3 are bound to M by coordination bonds and wherein R sub 1 and R sub 2 may be the same or different, but if the same are different from R sub 3 ; with the proviso that the complex does not have the formula M(byp) sub 2 (dppz).

2. A complex of claim 1, wherein M is Ru, Rh, or Co.

3. A complex of claim 1, wherein R sub 1 and R sub 2 are the same.

4. A complex of claim 3 having the formula M(phen) sub 2 (phi), M(byp) sub 2 (phi), M(phi) sub 2 (bpy), M(phi) sub 2 (4,4'diphenylbipyridine), M(bis 4,4'methyl bipyridylate) sub 2 (phi), M(bis 4,4'bipyridylamide) sub 2 (phi), M(bpy) sub 2 (phen), M(phen) sub 2 (bpy), M(phen) sub 2 (flone),

M(bpy) sub 2 (DIP), M(phen) sub 2 (DIP), M(DIP) sub 2 (phen), M(phen) sub 2 (dppz), M(DIP) sub 2 (dppz), or M(dppz) sub 2 (phen).

5. A complex of claim 4, wherein M is Ru, Rh, or Co.

6. A complex of claim 5, wherein M is Ru.

7. A complex of claim 5, wherein M is Rh.

8. A coordination complex or salt thereof which is spectroscopically or photoactively determinable when bound to DNA having the formula [See structure in original document] wherein M is Ru, Rh, Co, Fe, Cr, Cu, Zn, Cd, or Pd, and each of R sub 1, R sub 2, and R sub 3 is ethylenediamine, bipyridine, 2,2'-bipyridine (bpy), 4,4'diphenyl bipyridine, bis 4,4'methyl bipyridylate, bis 4,4'bipyridylamide, phenanthroline, 1,10-phenanthroline (phen), 4,7-diamino-1,10-phenanthroline, 3,8-diamino-1,10-phenanthroline, 4,7-diethylenediamine-1,10-phenanthroline, 3,8-diethylenediamine-1,10-phenanthroline, 4,7-dihydroxyl-1,10-phenanthroline, 3,8-dihydroxyl-1,10-phenanthroline, 4,7-dinitro-1,10-phenanthroline, 3,8-dinitro-1,10-phenanthroline, 4,7-diphenyl-1,10phenanthroline (DIP), 3,8-diphenyl-1,10-phenanthroline, 4,7-dispermine-1,10-phenanthroline, 3,8-dispermine-1,10-phenanthroline, 5-nitrophenanthroline (5-NO sub 2 phen), 3,4,7,8-tetramethylphenanthroline (TMP), diazafluorene-9-one, 4,5-diazafluorene-9-one (flone), phenanthrenequinonediimine, 9,10-phenanthrenequinonediimine (phi), dipyridophenazine, or 3,2-dipyridophenazine (dppz); wherein R sub 1, R sub 2, and R sub 3 are bound to M by coordination bonds, provided that at least one of R sub 1, R sub 2, or R sub 3 is dipyridophenazine, of 3,2-dipyridophenazine (dppz); with the proviso that the complex does not have the formula M(byp) sub 2 (dppz).

9. A complex of claim 8, wherein M is Ru.

10. A complex of claim 9 having the formula Ru(phen) sub 2 (dppz) sup 2+.

11. A complex of claim 9 having the formula Ru(DIP) sub 2 (dppz) sup 2+.

12. A complex of claim 9 having the formula Ru(dppz) sub 2 (phen) sup 2+.

13. A complex of claim 9 having the formula Ru(dppz) sub 2 (bpy) sup 2+.

14. A coordination complex or salt thereof which is spectroscopically or photoactively determinable when bound to DNA having the formula [See structure in original document] wherein M is Ru or Rh and R is 9-10-phenanthrenequionediimine, 5-nitrophenanthroline, or 3,2-dipyridophenazine.

15. The optically resolved delta isomer of the complex of claim 14.

16. The optically resolved lambda isomer of the complex of claim 14.

17. A pharamceutical composition which comprises an amount of the complex Rh(DIP) sub 3 effective to inhibit the activity of human immunodeficiency virus and a pharmaceutically acceptable carrier.

18. A method of inhibiting the growth of HIV in HIV-infected cells which comprises contacting the cells with an amount of an Rh(DIP) sub 3 complex effective to inhibit the growth of HIV.

? t s2/5/2,13,18,82,89,90,93

2/5/2 (Item 2 from file: 2)
DIALOG(R)File 2:INSPEC

04385405 INSPEC Abstract Number: A9310-8715M-004
Title: New developments in Raman spectroscopy of biological systems
Author(s): Fabian, H.; Anzenbacher, P.
Author Affiliation: Max-Delbruck-Center for Molecular Med., Berlin-Buch, Germany
Journal: Vibrational Spectroscopy vol.4, no.2 p.125-48
Publication Date: 14 Jan. 1993 Country of Publication: Netherlands
CODEN: VISPEK ISSN: 0924-2031
U.S. Copyright Clearance Center Code: 0924-2031/93/$06.00
Language: English Document Type: Journal Paper (JP)
Treatment: Bibliography (B); Practical (P); Experimental (X)
Abstract: The authors review developments in Raman spectroscopy of biological materials. After a brief description of technical aspects of the instrumentation and procedures the broad range of biological systems studied by many scientists using a wide variety of techniques is discussed. Illustrative examples of experimental studies are given to indicate the different possibilities and the present status of Raman spectroscopy in various fields of biochemistry and biomedicine. (322 Refs)
Descriptors: molecular biophysics; Raman spectroscopy; reviews
Identifiers: biological systems; Raman spectroscopy; instrumentation; biochemistry; biomedicine
Class Codes: A8715M (Interactions with radiations at the biomolecular level); A0130R (Reviews and tutorial papers; resource letters)

2/5/13 (Item 13 from file: 2)
DIALOG(R)File 2:INSPEC

01417166 INSPEC Abstract Number: A79092014
Title: Resonance Raman spectroscopy
Author(s): Morris, M.D.; Wallan, D.J.
Author Affiliation: Dept. of Chem., Univ. of Michigan, Ann Arbor, MI, USA
Journal: Analytical Chemistry vol.51, no.2 p.182A-3, 185A-6, 188A, 190A, 192A
Publication Date: Feb. 1979 Country of Publication: USA
CODEN: ANCHAM ISSN: 0003-2700
Language: English Document Type: Journal Paper (JP)
Treatment: General, Review (G)
Abstract: Resonance Raman spectroscopy possesses many features that make it attractive to the analytical chemist. These properties are outlined. However, problems of sample fluorescence have limited its practical applications. The authors outline the theory of resonance Raman spectroscopy and review the published analytical applications. They also describe the most promising approach to fluorescence rejection, coherent resonance Raman spectroscopy, and summarize the current applications and the prospects for the future. (51 Refs)
Descriptors: Raman spectroscopy; reviews; spectrochemical analysis
Identifiers: sample fluorescence; resonance Raman spectroscopy; fluorescence rejection; coherent resonance Raman spectroscopy; analytical chemistry uses
Class Codes: A0765 (Optical spectroscopy and spectrometers); A8280D (Electromagnetic radiation spectrometry)

2/5/18 (Item 18 from file: 2)
DIALOG(R)File 2:INSPEC

00504140 INSPEC Abstract Number: A73026745
Title: Raman spectroscopy of biological molecules: a review
Author(s): Koenig, J.L.
Author Affiliation: Case Western Reserve Univ., Cleveland, OH, USA
Journal: Journal of Polymer Science, Macromolecular Reviews vol.6 p.59-177
Publication Date: 1972 Country of Publication: USA
CODEN: JPDMAJ ISSN: 0076-2083
Language: English Document Type: Journal Paper (JP)
Treatment: General, Review (G)
(61 Refs)
Descriptors: organic compounds; Raman spectra of organic substances; reviews
Identifiers: Raman spectroscopy; biological molecules
Class Codes: A3620K (Electronic structure and spectra)

2/5/82 (Item 1 from file: 94)
DIALOG(R)File 94:JICST-EPlus

03737553 JICST ACCESSION NUMBER: 97A0420786 FILE SEGMENT: JICST-E
Quantitative analysis of trace biological molecules by Raman spectroscopy.
DOU X (1); OZAKI YUKIHIRO (2)
(1) Kyoto Daiichi Kagaku Co., Ltd.; (2) Kwansei Gakuin Univ., Sch. of Sci.
Oyo Butsuri, 1997, VOL.66,NO.4, PAGE.345-350, FIG.9, REF.12
JOURNAL NUMBER: F0252AAQ ISSN NO: 0369-8009 CODEN: OYBSA
UNIVERSAL DECIMAL CLASSIFICATION: 57.08
LANGUAGE: Japanese COUNTRY OF PUBLICATION: Japan
DOCUMENT TYPE: Journal
ARTICLE TYPE: Review article
MEDIA TYPE: Printed Publication
ABSTRACT: Raman spectroscopy has been employed extensively to investigate the structure, reaction mechanism and excitation stases of various types of materials. Recently, the remarkable progress in lasers and detectors has increased understanding of the applications of Raman spectroscopy. In this review, we report on the Raman analysis of trace metabolic materials, by presenting our recent studies as examples. In particular, from the viewpoint of new spectroscopic techniques, we discuss the highly sensitive quantitative analysis of biological materials using anti-Stokes Raman spectroscopy, near-infrared Raman spectroscopy and surface-enhanced Raman spectroscopy, which are all powerful in avoiding or rejecting fluorescence. The potential application use of Raman spectroscopy in clinical chemistry is also described in this review. (author abst.)
DESCRIPTORS: Raman spectrometry; SERS spectroscopy; CARS spectroscopy; biological sample; metabolite; glucose; urea; stretching vibration(molecule); microanalysis; immunoassay; enzymatic analysis
BROADER DESCRIPTORS: spectrochemical analysis; instrumental analysis; analysis(separation); analysis; Raman spectroscopy; spectroscopy; laser spectroscopy; sample; aldose; reducing sugar; carbohydrate; hexose; urea compound; molecular vibration; oscillation; molecular motion; motion; bioassay; biochemical analysis; chemical analysis
CLASSIFICATION CODE(S): EA03010K

2/5/89 (Item 2 from file: 636)
DIALOG(R)File 636:IAC Newsletter DB(TM)

01004901
TRENDS IN INSTRUMENTATION -- A REVIEW OF LASER BASED MICROCHEMICAL ANALYSIS
CHEMICAL MONITOR January 00, 1991 V. 7 NO. 1
WORD COUNT: 206
PUBLISHER: Angelo Tulumello Ph.D.

This is a review of the various ways that lasers are used in microchemical analysis. The usual procedure is to separate sample components using a chromatographic procedure and then use the laser as a source in an optical measurement. The authors report their work as well as a review of other researchers methods of laser based chemical analysis. To perform an analysis on the DNA chain the authors were able to add a fluorescent material to the DNA components. They then performed a column electrophoresis to separate the components. The detectors used have of detection limits of 0.001 attomoles, which is equivalent to 600 atoms. (1 attomole = 10 to the minus 18 moles). With this level of sensitivity, it may be of interest to reference the separation process. The separation process is a modification of gel chromatography. It occurs on an electrophoretic gel. The columns are filled with a polyacrylamide gel. They are 1 meter long and 50 micron-i.d. Flow occurs when 22-kV is placed across them. Examples of many other laser optical microchemical methods are given. Many are extensions, modifications and improvements on classical methods, such a refractometry and Raman spectroscopy. **Dovichi, N.J. Review of Scientific Instruments, Vol. 61, No. 12, pp. 3653-3667, December (1990)**

INDUSTRY: Instrumentation (IN)

2/5/90 (Item 1 from file: 653)
DIALOG(R)File 653:US Pat.Fulltext

01542307
Utility
QUALITATIVE AND QUANTITATIVE ANALYSIS USING RAMAN SCATTERING
[For determining the composition of an unknown sample]

PATENT NO.: 4,620,284
ISSUED: October 28, 1986 (19861028)
INVENTOR(s): Schnell, Robert P., Deerfield, IL (Illinois), US (United States of America)
Sampson, Robert W., Wayne, IL (Illinois), US (United States of America)
Pacanowski, Ronald F., Hoffman Estates, IL (Illinois), US (United States of America)
Bruggema, Donald J., Wheeling, IL (Illinois), US (United States of America)
ASSIGNEE(s): UOP Inc , (A U.S. Company or Corporation), Des Plaines, IL (Illinois), US (United States of America)
[Assignee Code(s): 87900]

EXTRA INFO: Assignment transaction [Reassigned], recorded September 21, 1988 (19880921)
Assignment transaction [Reassigned], recorded April 27, 1989 (19890427)

POST-ISSUANCE ASSIGNMENTS

ASSIGNEE(s): UOP, DES PLAINES, IL, A NY GENERAL PARTNERSHIP
Assignor(s): KATALISTIKS INTERNATIONAL, INC., A CORP. OF MD -- signed: 09/16/1988
Recorded: September 21, 1988 (19880921)
Reel/Frame: 5006/0782
Brief: ASSIGNMENT OF ASSIGNOR'S INTEREST
Rep.: UNION CARBIDE CORPORATION 39 OLD RIDGEBURY ROAD DANBURY, CT 06817-0001
ASSIGNEE(s): UOP, DES PLAINES, IL A GENERAL PARTNERSHIP OF NY
Assignor(s): UOP INC. -- signed: 08/22/1988
Recorded: April 27, 1989 (19890427)
Reel/Frame: 5077/0005
Brief: ASSIGNMENT OF ASSIGNOR'S INTEREST
Rep.: THOMAS K. MCBRIDE UOP 25 EAST ALGONQUIN RD. DES PLAINES, IL 60017-5017

APPL. NO.: 6-566,842
FILED: December 29, 1983 (19831229)
U.S. CLASS: 364-498 cross ref: 356-301
INTL CLASS: [4] G06F 15-20; G01J 3-44
FIELD OF SEARCH: 364-499; 364-498; 364-497; 364-496; 364-525; 356-301; 356-306; 356-307

References Cited

U.S. PATENT DOCUMENTS

2,527,121	10/1950	Dudenbostel	356-301
2,527,122	10/1950	Heigl et al.	356-301
2,940,355	6/1960	Cary	356-301
3,414,354	12/1968	Siegler	356-301
3,556,659	1/1971	Hawes	356-301
3,625,613	12/1971	Abell et al.	356-301
3,723,007	3/1973	Leonard	356-301
3,820,897	6/1974	Roess	356-301
4,030,827	6/1977	Delhaye et al.	356-301
4,068,953	1/1978	Harney et al.	356-301
4,127,329	11/1978	Chang et al.	356-301
4,195,930	4/1980	Delhaye et al.	356-301
4,267,572	5/1981	Witte	364-498
4,270,864	6/1981	Barrett et al.	356-301
4,365,303	12/1982	Hannah et al.	364-498
4,397,556	8/1983	Muller	356-301
4,505,586	3/1985	Tochigi et al.	356-301

OTHER REFERENCES

Analytical Chemistry, vol. 21, No. 5, May 1949, pp. 554-559, "Determination of Total Olefins and Total Aromatics", by J. J. Heigl et al.

Proceedings of the American Petroleum Institute, vol. 27-28, 1948, pp. 95-105, "Determination of Total Olefins and Total Aromatics", by J. J.

Heigl et al.

Report of a Conference held by The Institute of Petroleum in London on Oct. 28-29, 1954 entitled "Molecular Spectroscopy".

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ABSTRACT

Methods and apparatus are provided for qualitative and quantitative analysis utilizing the Raman effect. Analyses are obtainable without exercise of human judgment or human interpretation. Analyses may be obtained on-line in the field or in a laboratory. A wide range of fluids and solids are capable of rapid routine analysis without major adjustment of equipment. An analysis is obtained by comparing a Raman spectrum of the unknown sample to Raman spectra of samples whose analysis is known. The known Raman spectra are stored in computing means in digital form and the comparison is accomplished by the computing means.

We claim as our invention:

1. A method for determining the composition of an unknown sample comprising:

(a) producing a beam of photons which is substantially monochromatic and impinges on the unknown sample;

(b) collecting photons scattered by the unknown sample into a stream of scattered photons;

(c) resolving the photon stream into its component frequencies to form a Raman spectrum of the unknown sample;

(d) providing said unknown sample Raman spectrum to a computer;

(e) providing to the computer reference spectra obtained in the same manner as said unknown spectrum, where the reference spectra are of reference samples whose composition is known; and,

(f) identifying substances present in the unknown sample by comparing said unknown spectrum to the reference spectra, said comparison being accomplished by utilizing the computer and comprising the following steps:

(i) inspecting the unknown spectrum and selecting a plurality of separate spectral analysis regions;

(ii) determining a size characteristic associated with each of said spectral analysis regions of the unknown spectrum;

(iii) searching the reference spectra and choosing those reference spectra having in the selected spectral analysis regions features corresponding to those of the selected spectral analysis regions of the unknown spectrum and size characteristics substantially identical to those of the selected spectral analysis regions of the unknown spectrum;

(iv) if more than one reference spectrum is chosen, repeating steps (f)(i), (f)(ii), and (f)(iii), selecting additional spectral analysis regions, until only one reference spectrum is chosen, the substances present in said one chosen reference spectrum being present in the unknown samples;

(v) if no reference spectrum is chosen, establishing a number of working

hypotheses, each hypothesis being that the unknown sample consists of a different combination of the reference samples which exhibited the spectra chosen to have features corresponding to those of the selected spectral regions of the unknown spectrum;

(vi) testing each working hypothesis by combining the spectra of the hypothesis to produce a single hypothetical spectrum and comparing it to the unknown spectrum;

(vii) discarding each working hypothesis which is not substantially identical to the unknown spectrum; and,

(viii) if more than one working hypothesis has not been discarded, repeating steps (f)(v) through (f)(viii), selecting additonal spectral analysis regions, until only one working hypothesis has not been discarded, the unknown sample composition then being that of said one remaining working hypothesis.

2. The method of claim 1 further characterized in that said size characteristic is the height of the highest peak of the spectral analysis region.

3. The method of claim 1 further characterized in that said size characteristic is the area of the spectral analysis region.

4. The method of claim 1 further characterized with respect to step (f)(vi) in that said testing is accomplised by:

(a) for each working hypothesis, establishing a set of equations consisting of one equation associated with each selected region of the unknown spectrum, which equation describes the area of the region in terms of concentrations of the reference samples and areas of reference spectra regions; and,

(b) attempting to solve each set of equations and concluding that each working hypothesis whose set of equations cannot be completely solved or yields unreal numbers is not substantially identical to the unknown spectrum.

5. The method of claim 4 further characterized in that said equation associated with each region is of the formX sub 1 C sub 1 +X sub 2 C sub 2 + . . . +X sub n C sub n =A,

where

C sub 1, C sub 2, . . . C sub n =the concentration of the substance of reference samples 1, 2, . . . n in the hypothetical combination of reference samples,

X sub 1, X sub 2, . . . X sub n =the areas of those regions in each of the reference spectra of the hypothetical combination, and

A=the area of the region of the unknown spectrum.

6. A method for performing a quantitative analysis for preselected substances of an unknown sample comprising:

(a) producing a beam of photons which is substantially monochromatic and impinges on the unknown sample;

(b) collecting photons scattered by the unknown sample into a stream of scattered photons;

(c) resolving the photon stream into its component frequencies to form a Raman spectrum of the unknown sample;

(d) providing said unknown sample Raman spectrum to a computer;

(e) providing to the computer reference spectra obtained in the same manner as said unknown spectrum, where the reference spectra are of reference samples whose quantitative composition is known and where each reference sample is comprised of at least one of said preselected substances; and,

(f) identifying substances present in the unknown sample by comparing said

unknown spectrum to the reference spectra, said comparison being accomplished by utilizing the computer and comprising the following steps:

(i) inspecting the reference spectra and selecting a plurality of separate spectral analysis regions;

(ii) determining the areas of the selected regions for each reference spectrum and for the unknown spectrum;

(iii) establishing a relationship between said reference spectra region areas and concentrations of said preselected substances in said reference samples; and,

(iv) determining the concentrations of said preselected substances in said unknown sample by applying the relationship established in step (f)(iii) to the unknown spectrum region areas.

7. The method of claim 6 further characterized with respect to step (f) in that said relationship is established and said concentrations determined by:

(a) selecting a number of spectral analysis regions equal to the number of said preselected substances;

(b) determining the areas of the selected regions for each reference spectrum and for the unknown spectrum and calculating area fractions for the reference spectra and for the unknown spectrum;

(c) establishing a set of equations for each reference sample where the number of equations in each set is equal to the number of said preselected substances and each equation describes the concentration of one preselected substance in terms of its contributions to region areas, each equation having the formX=C sub 1x A sub 1 +C sub 2x A sub 2 + . . . +C sub nx A sub n,

where

X represents the concentration fraction of the preselected substance,

A sub 1, A sub 2, . . . A sub n are area fractions of the selected regions of the spectrum of the reference sample where n equals the number of regions, and

C sub 1x, C sub 2x, . . . C sub nx are coefficients associated with the contributions of the preselected substances to the regions;

(d) solving all of the equations established in step (c) for said coefficients;

(e) establishing one set of equations for the unknown sample as was done in step (c) for each reference sample; and,

(f) solving said unknown sample equations for the concentrations of the preselected substances, using the coefficients determined in step (d).

8. The method of claim 6 further characterized with respect to steps (f)(iii) and (f)(iv) in that said relationship is established and said concentrations determined by:

(a) expressing said reference sample concentrations in terms of concentration fractions and arranging the concentration fractions in a concentration fraction matrix, according to said reference samples and said preselected substances;

(b) calculating area fractions from said reference spectra region areas and arranging the area fractions into an area fraction matrix, according to said reference samples and the selected regions;

(c) determining a transpose matrix, which is the transpose of the area fraction matrix;

(d) forming a mathematical quantity using said matrices, as follows: [See equation in original document] (e) solving said mathematical quantity to yield a matrix, which consists of correlation coefficients, arranged according to the selected regions and said preselected substances;

(f) calculating area fractions from said unknown spectrum region areas and arranging the area fractions in a matrix; and,

(g) multiplying said correlation coefficient matrix by the matrix formed

of said unknown spectrum area fractions to obtain a product which is a concentration fraction matrix which expresses the concentrations of the preselected substances in said unknown sample.

9. The method of claim 6 further characterized in that the substances comprising said unknown sample are paraffins, naphthenes, and aromatics.

10. The method of claim 6 further characterized in that said beam of photons is from a laser source.

11. The method of claim 6 further characterized in that the wave lengths of said beam of photons are closely centered about a value of 6328 angstroms.

12. The method of claim 6 further characterized in that photons are removed from said stream of photons before it is resolved to form a spectrum, the removed portion consisting of photons at the same frequency as said beam of photons and at a higher frequency than the frequency of said beam of photons.

13. The method of claim 6 further characterized in that composite reference spectra are used in performing said comparison, a composite reference spectrum being prepared for each reference sample by providing a plurality of spectra of each reference sample to the computer and averaging each of said plurality of reference spectra.

14. The method of claim 6 further characterized in that a portion of said Raman spectrum is removed and not provided to the computer, such portion consisting of Rayleigh scattered light and the anti-Stokes lines.

15. The method of claim 6 further characterized in that said unknown spectrum and said reference spectra are adjusted to substantially remove false information before said comparison is accomplished.

16. The method of claim 15 further characterized in that said false information comprises a background spectrum, which is obtained in the same general manner as a sample spectrum but with said beam of photons interrupted, and said adjustment to remove false information is accomplished by subtracting the background spectrum intensity from the sample spectrum intensity at each frequency.

17. The method of claim 15 further characterized in that said false information comprises sample fluorescence and stray photons and said adjustment to remove false information is accomplished by means of establishing baselines and discarding that portion of the spectrum which is below the baselines.

18. Apparatus for determining the composition of an unknown sample comprising:

(a) means for producing a beam of photons which is substantially monochromatic and impinges on the unknown sample;

(b) means for collecting photons scattered by the unknown sample into a stream of scattered photons;

(c) means for resolving the photon stream into its component frequencies to form a Raman spectrum of the unknown sample;

(d) means for converting said unknown sample Raman spectrum to digital form and transmitting said unknown spectrum to computing means;

(e) said computing means, which contain reference spectra obtained in the same manner as said unknown spectrum, where the reference spectra are of reference samples whose composition is known; and,

(f) means within the computing means for identifying substances present in the unknown sample by comparing said unknown spectrum to the reference

spectra, said computing means accomplishing said comparison by performing the following functions:

(i) inspecting the unknown spectrum and selecting a plurality of separate spectral analysis regions;

(ii) determining a size characteristic associated with each spectral analysis region of the unknown spectrum;

(iii) searching the reference spectra and choosing those reference spectra having in the selected spectral analysis regions features corresponding to those of the selected spectral analysis regions of the unknown spectrum and size characteristics substantially identical to those of the selected spectral analysis regions of the unknown spectrum;

(iv) if more than one reference spectrum is chosen, repeating functions (f)(i), (f)(ii), and (f)(iii), selecting additional regions, until only one reference spectrum is chosen, the substances present in said one chosen reference spectrum being present in the unknown sample;

(v) if no reference spectrum is chosen, establishing a number of working hypothesis, each hypothesis being that the unknown sample consists of a different combination of the reference samples which exhibited the spectra chosen to have features corresponding to those of the selected regions of the unknown spectrum;

(vi) testing each working hypothesis by combining the spectra of the hypothesis to produce a single hypothetical spectrum and comparing it to the unknown spectrum;

(vii) discarding each working hypothesis which is not substantially identical to the unknown spectrum; and,

(viii) if more than one working hypothesis has not been discarded, repeating functions (f)(v) through (f)(viii), selecting additional regions, until only one working hypothesis has not been discarded, the unknown sample composition then being that of said one remaining working hypothesis.

19. The apparatus of claim 18 further characterized with respect to function (f)(vi) in that said testing is accomplished by:

(a) for each working hypothesis, establishing a set of equations consisting of one equation associated with each selected region of the unknown spectrum, which equation describes the area of the region in terms of concentrations of the reference samples and areas of reference spectra regions; and

(b) attempting to solve each set of equations and concluding that each working hypothesis whose set of equations cannot be completely solved or yields unreal numbers is not substantially identical to the unknown spectrum.

20. The apparatus of claim 19 further characterized in that said equation associated with each region is of the formX sub 1 C sub 1 +X sub 2 C sub 2 + . . . +X sub n C sub n =A,

Where

C sub 1, C sub 2, . . . C sub n =the concentration of the substance of reference samples 1, 2, . . . n in the hypothetical combination of reference samples,

X sub 1, X sub 2, . . . X sub n =the areas of those regions in each of the reference spectra of the hypothetical combination, and

A=the area of the region of the unknown spectrum.

21. Apparatus for performing a quantitative analysis for preselected substances of an unknown sample comprising:

(a) means for producing a beam of photons which is substantially monochromatic and impinges on the unknown sample;

(b) means for collecting photons scattered by the unknown sample into a

stream of scattered photons;
(c) means for resolving the photon stream into its component frequencies to form a Raman spectrum of the unknown sample;
(d) means for converting said unknown sample Raman spectrum to digital form and transmitting said unknown spectrum to computing means;
(e) said computer means, which contain reference spectra obtained in the same manner as said unknown spectrum, where the reference spectra are of reference samples whose quantitative composition is known and where each reference sample is comprised of at least one of said preselected substances; and,
(f) means within the computer for identifying substances present in the unknown sample by comparing said unknown spectrum to the reference spectra, said computer accomplishing said comparison by performing the following functions:
(i) inspecting the reference spectra and selecting a plurality of separate spectral analysis regions;
(ii) determining the areas of the selected regions for each reference spectrum and for the unknown spectrum;
(iii) establishing a relationship between said reference spectra region areas and concentrations of said preselected substances in said reference sample; and
(iv) determining the concentrations of said preselected substances in said unknown sample by applying the relationship established in function (f)(iii) to the unknown spectrum region areas.

22. The apparatus of claim 21 further characterized with respect to element (f) in that said relationship is established and said concentrations determined by the following functions:
(a) selecting a number of spectral analysis regions equal to the number of said preselected substances;
(b) determining the areas of the selected regions for each reference spectrum and for the unknown spectrum and calculating area fractions;
(c) establishing a set of equations for each reference sample where the number of equations in each set is equal to the number of said preselected substances and each equation describes the concentration of one preselected substance in terms of its contributions to region areas, each equation having the formX=C sub 1x A sub 1 +C sub 2x A sub 2 + . . . +C sub nx A sub n,
where
X represents the concentration fractions of the preselected substance,
A sub 1, A sub 2, . . . A sub n are area fractions of the selected regions of the spectrum of the reference sample where n equals the number of regions, and
C sub 1x, C sub 2x, . . . C sub nx are coefficients associated with the contributions of the preselected substances to the regions;
(d) solving all of the equations established in function (c) for said coefficients:
(e) establishing one set of equations for the unknown sample as was done in function (c) for each reference sample; and,
(f) solving said unknown sample equations for the concentrations of the preselected substances, using the coefficients determined in function (d).

23. The apparatus of claim 21 further characterized with respect to functions (f)(iii) and (f)(iv) in that said relationship is established and said concentrations determined by:
(a) expressing said reference sample concentrations in terms of concentration fractions and arranging the concentration fractions in a concentration fraction matrix, according to said reference samples and said preselected substances;
(b) calculating area fractions from said reference spectra region areas

and arranging the area fractions into an area fraction matrix, according to said reference samples and the selected regions;
(c) determining a transpose matrix, which is the transpose of the area fraction matrix;
(d) forming a mathematical relationship using said matrices, as follows: [See equation in original document] (e) solving said mathematical quantity to yield a matrix, which consists of correlation coefficients, arranged according to the selected regions and said preselected substances;
(f) calculating area fractions from said unknown spectrum region areas and arranging the area fractions in a matrix; and,
(g) multiplying said correlation coefficients matrix by the matrix formed of said unknown spectrum area fractions to obtain a product which is a concentration fraction matrix which expresses the concentrations of the preselected substances in said unknown sample.

24. The apparatus of claim 21 further characterized in that the substances comprising said unknown sample are paraffins, naphthenes, and aromatics.

25. The apparatus of claim 21 further characterized in that said beam of photons is from a laser source.

26. The apparatus of claim 21 further characterized in that the wave lengths of said beam of photons are closely centered about a value of 6328 angstroms.

27. The apparatus of claim 21 further comprising means for removing photons from said stream of photons before it is resolved to form a spectrum, the removed portion consisting of photons at the same frequency as said beam of photons and at a higher frequency than the frequency of said beam of photons.

28. The apparatus of claim 21 further comprising means for using composite reference spectra in performing said comparison, a composite reference spectrum being prepared for each reference sample by providing a plurality of spectra of each reference sample to said computer means and averaging each of said plurality of reference spectra.

29. The apparatus of claim 21 further comprising means for removing a portion of said Raman spectrum, such portion consisting of Rayleigh scattered light and the anti-Stokes lines.
30. The apparatus of claim 21 further comprising means for adjusting said unknown spectrum and said reference spectra to substantially remove false information before said comparison is accomplished.

31. The apparatus of claim 30 further characterized in that said spectrum adjusting means comprises means for providing to said computer means a background spectrum for use in accomplishing said adjustment to remove false information, said background spectrum being obtained in the same general manner as a sample spectrum but with said beam of photons interrupted, and said adjustment to remove false information being accomplished by subtracting the background spectrum intensity from the sample spectrum intensity at each frequency.

32. The apparatus of claim 30 further comprising means for substantially removing those portions of the spectra which comprise sample fluorescence and stray photons by means of establishing baselines and discarding that portion of the spectrum which is below the baselines.

2/5/93 (Item 1 from file: 53)
DIALOG(R)File 53:FOODLINE(R): Food Science & Technology

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UV Resonance Raman spectroscopic detection and identification of bacteria and other microorganisms.
Nelson W H; Sperry J F
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Nelson W H
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ABSTRACT: Raman spectroscopy was first introduced over sixty years ago as a method for studying vibrations and rotations of small molecules, but was not widely used owing to a number of practical problems. Advances in the last twenty-five years have widened the applications of this analytical technique. One major advance has come through the use of resonance Raman spectroscopy. This review describes the use of resonance Raman, particularly UV resonance Raman, spectroscopy for the detection and identification of microorganisms. Consideration is given to the theory and mechanism of Raman spectra; the properties of bacterial macromolecules such as proteins, purines, pyrimidines and nucleic acids; UV excitation of bacterial molecules; the effects of cultural conditions; determination of GC/AT ratios; and the study of bacterial spores, pollen and viruses. Figures showing the UV resonance spectra of bacteria include Ps. fluorescens, E. cloacae, E. coli, S. epidermidis, P. mirabilis, Bacillus sp. and cyanobacteria.
SECTION HEADING: MICROBIOLOGY
DESCRIPTORS: BACTERIA; BACTERIAL SPORES; COMPOSITION; COMPOUNDS; DETECTION; IDENTIFICATION; MECHANISMS; MICROBIAL SPORES; MICROORGANISMS; RAMAN; RAMAN RESONANCE SPECTROSCOPY; RAMAN SPECTROSCOPY; RESONANCE; REVIEW; SPECTRA; SPECTROSCOPY; SPORES; UV RADIATION; UV SPECTRA; UV SPECTROSCOPY; VIRUSES
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